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Simulation and analysis of highly sensitive MEMS cantilever designs for "in vivo label free" biosensing

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Abstract

In Bio-MEMS applications, low mass loading of biomolecules on rectangular microcantilever beam surface gives negligible deflection at it's free end and poor sensitivity corresponding to the lower concentration of analyte. This paper presents three new microcantilever designs for biosensing, which hold promises for better deflection and higher sensitivity. The proposed designs provide the free end deflection nearly twice as the conventional rectangular beam. The FEM software ANSYS 12.1 is carried out to analyze the deflection of the proposed microcantilever designs.

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Keywords: microcantilever beam; in vivo analysis; biosensor.

1. Introduction

Micro electro mechanical system incorporates highly sensitive miniaturized devices such as sensor and actuator which have high throughput, high performance, low cost and easy fabrication. These miniaturized devices are widely used in various sensing and switching applications. Mainly three type of biosensing transduction method are used: potentiometric, amperometeric and microcantilever biosensor. In potentiometric biosensor, the detection of biomolecules is achieved by the measurement of change in current value from source unit to drain unit. This method is limited to only the detection of charge molecules like DNA. In amperometric biosensor, electrodes are used for biomolecular detection. This method of biosensing is also limited to charge molecules. The facility of multi agent detection is not feasible in both these biosensing method. In microcantilever based biosensor, the concentration of

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biomolecules present at the cantilever surface can be achieved by the stress generated inside the cantilever or by the frequency difference. MEMS cantilevers for bio sensing, are adequate to convert biomolecular event into specific measurable quantity. The applications of bio MEMS microcantilevers are pH detection [5], bio-recognition activities analysis and mass detection [1], antigen-antibody reaction [9], triglyceride detection [4], monolayers molecules attogram detection [3], biomolecular analysis such as DNA [2], monomethylmercury detection [6], triaxial tactile measurement [7] and glucose sensing using poly-silicon-based CMOS [8]. The main advantage of microcantilever biosensing is multiagent detection with the help of microcantilever array.

MEMS cantilever gives quick and exact response based on biomolecular activities as compare to the conventional cantilever design. The small size and less amount of analyte required in detection compose MEMS cantilever more applicable in lower concentration biosensing. In such cantilever, the settling time of biomolecule, which is mainly taken by the analyte molecule to settle down on the sensor surface, decreases and provides rapid detection of biomolecules. There are two operating mode of cantilever: static and dynamic. In former, the deflection is measured by the pressure produced by the biomolecules on the cantilever surface. In later, the concentration of biomolecules is measured by detecting the change in oscillating frequency with respect to the change in mass, where applied sinusoidal voltage is kept constant. The deflection at the micro cantilever beam can be monitored by various methods namely, optical reflection, capacitive and electron tunneling, interferometric and piezoelectric based detection. The optical reflection is most effective method for deflection detection.

Bio-molecular analysis requires four elements: a target analyte, a specific bio receptor, a sensing unit and a detecting unit, as shown in Fig. 1(a). In “in vivo analysis”, sensing unit need to be very sensitive. If the concentration of target analyte solution is small then it produces less pressure at the sensor surface. This less pressure generated by biomolecular event is unable to sense by the conventional rectangular microcantilever based sensor. This paper focuses on the high sensitivity and better deflection at the microcantilever free end for low mass loading. Based on this objective, new microcantilever designs with better efficiency and sensitivity are proposed in this paper. For analyzing the deflection value, the surface area of all proposed designs is kept constant ($5000\mu m^2$). The length and thickness of the proposed designs are also same as the conventional rectangular microcantilever beam design.

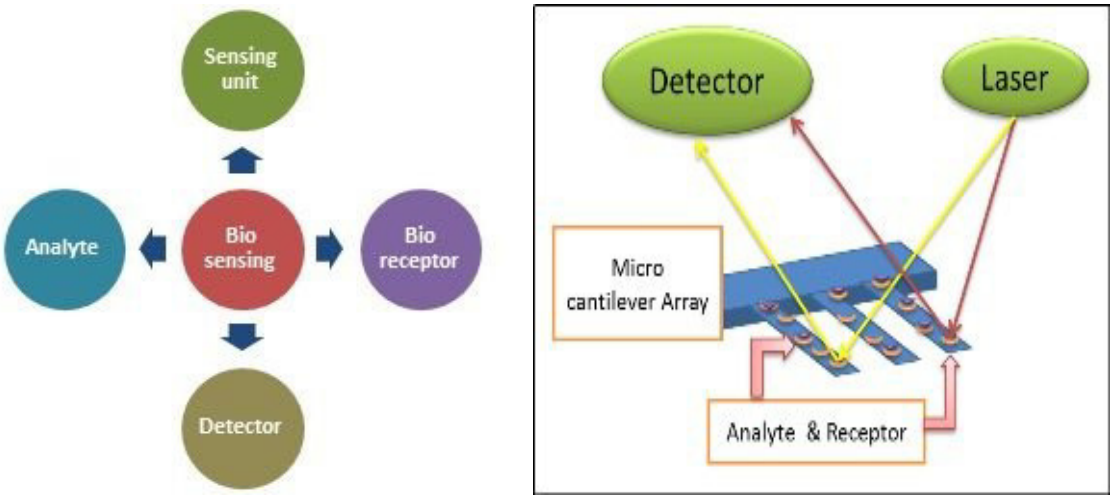

Fig. 1. (a) Basic elements of biosensing ; (b) Cantilever sensor setup for biosensing

Fig. 1(b) represents the microcantilever biosensing arrangement with beam array. The activities of biomolecules placed on microcantilever surface can be monitored with the help of laser and photo detector. Various types of analyte and bioreceptor can be analyzed with the help of different beams of microcantilever array.

2. Theory and operating principle

The principle of Bio-MEMS cantilever sensor is mainly based on the method of functionalization. In this method, bioreceptors are coated on the microcantilever surface to make it biosensitive. The biochemical reaction between the applied analyte and the bioreceptor can be observed by the deformation of microcantilever geometry. This deformation may be in the form of upward or downward deflection, which depends on the internal stress of the beam. For the rectangular microcantilever beam the free end deflection increases with the increment in beam length and decrement in beam thickness [9]. Materials which are used for the microcantilever design also effect it's free end deflection [9]. More elastic material gives more deflection at the microcantilever free end. According to Hook's law the free end deflection for microcantilever beam is directly proportional to the applied load.

$$\delta \propto F \tag{1}$$

$$\delta = aF \tag{2}$$

Where, a =1/k, δ is the deflection at the cantilever free end & F is the force produced by the biochemical reaction between the analyte and bioreceptor. Parameter k is the spring constant which mainly depends on flexural rigidity. In static mode, the sensitivity of microcantilever beam can be defined as, the change in free end deflection for the change in mass loading on microcantilever surface. The expression for sensitivity can be written as;

Sensitivity = change in deflection /change in molecular pressure

The biosensor called as highly sensitive if it can able to convert small change in pressure (1Pa to 5Pa) into measurable free end deflection. By the integration method, the expression for free end deflection of the conventional rectangular microcantilever beam [10] can be written as;

$$\delta = \frac{qwl^4}{8EI} \text{ (in case of UDL force)} \tag{3}$$

$$\delta = \frac{Pl^3}{3EI} \text{ (in case of point load)} \tag{4}$$

Where 'q' and 'P' are the uniformly distributed and point load, respectively. E and I are the Young's modulus and moment of inertia for the rectangular beam. By the work reported in [10], the relation between point load and induced surface stress can be written as;

$$P = \frac{\sigma wt(1-\nu)}{l} \tag{5}$$

By the equation (4) and (5), in terms of pressure we can write the expression for the deflection at the free end of conventional rectangular microcantilever beam, which is as follows;

$$\delta = \frac{3pl^4}{2Et^3} \tag{6}$$

Where 'p' is the pressure generated by the biomolecules on the microcantilever surface. Parameter 'σ' and 'ν' represent the stress and Poisson ratio for the beam. In [10] the maximum surface stress generated by injection of myoglobin protein on eight cantilever array is 0.05 N/m. For the conventional rectangular microcantilever beam, which is shown in Fig. 2(a), if the value of length (l), width (w) and thickness (t) are 500 µm, 100 µm and 50 µm,

respectively, then the pressure produced by the surface stress (0.05 N/m) is 19.2 Pa. The deflection at the free end of the rectangular cantilever beam for this pressure is 0.11×10^{-9} m which is shown in Fig. 2(b).

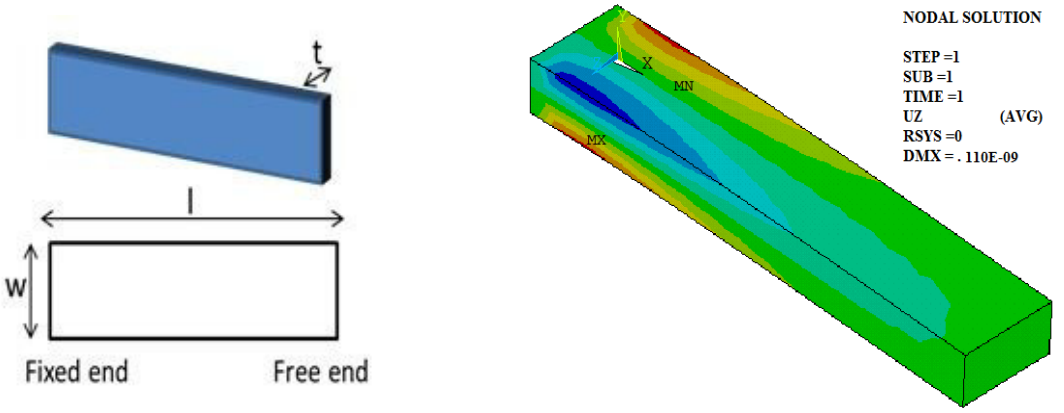

Fig. 2. (a) Rectangular microcantilever beam design; (b) It's free end deflection

3. Proposed microcantilever designs

We have proposed three new microcantilever designs for the detection of biomolecules. These beam designs can be effectively used in 'in vivo analysis', where mass loading on the cantilever surface is very less. In such application these designs give better (nearly double) deflection at the free end of microcantilever beam as compare to conventional rectangular one. A finite element method software ANSYS 12.1 is used for analyzing the deflection of the conventional rectangular and new proposed microcantilever beam designs. In this analysis element SOLID 20 node 186 is used for designing these beams. For defining the material properties, the density of material, Young's modulus and Poisson ratio are selected as 2.33 gm /cm^3, 130 GPa and 0.28, respectively.

3.1. Trapezoidal type microcantilever beam design

In this proposed design the width of beam increases linearly with the increment of beam length. The beam width at fixed end is narrow as compare to the width at the free end. This width variation from fixed end to free end gives the trapezoidal shape of microcantilever beam shown in Fig. 3(a). Parameter 'a' and 't' represent the complete length and thickness of this beam design. The width at fixed end and free end can be represented by the parameter 'b' and 'c', respectively. The value for parameter 'a', 'b' and 'c' are selected as 500 µm, 50 µm and 150 µm, respectively. The thickness 't' is 50 µm which is same as the rectangular beam.

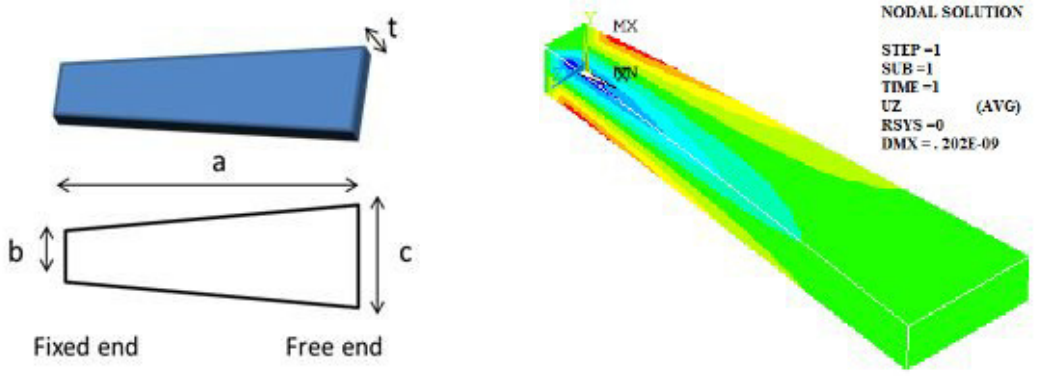

Fig. 3. (a) First proposed microcantilever beam design; (b) It's free end deflection

Fig. 3(b) shows the free end deflection of the proposed trapezoidal type microcantilever beam design with the surface area 50,000µm^2 and pressure 19.2Pa. Corresponding to this applied pressure, the trapezoidal beam design exhibits the free end deflection of 0.202×10^{-9} m.

3.2. Trapezoidal beam design with square step at fixed end

A square step of size 50×50×50 µm^3 is introduce at the fixed end of the trapezoidal shape design [discussed in previous section] such that the surface area and length are constant as the conventional rectangular beam. This gives the trapezoidal beam design with a square step at fixed end, as shown in Fig. 4(a). The length and thickness of this proposed beam are same as the rectangular beam. Parameter 'd', 'a' and 't' represent the length of square step, length of complete beam, and thickness of beam, respectively. The width of beam at the fixed end and free end of beam can be represented by parameter 'b' and 'c', respectively. The value for parameter 'a', 'b', 'c' and 'd' is selected as 500 µm, 50 µm, 161 µm and 50 µm, respectively. The thickness 't' is 50 µm which is same as the rectangular beam.

Fig. 4(b) shows the deflection at the free end of this proposed microcantilever design with constant surface area (50,000µm^2) and pressure (19.2Pa). The design gives the deflection of 0.231×10^{-9} m which is approximately twice as the rectangular microcantilever beam's deflection.

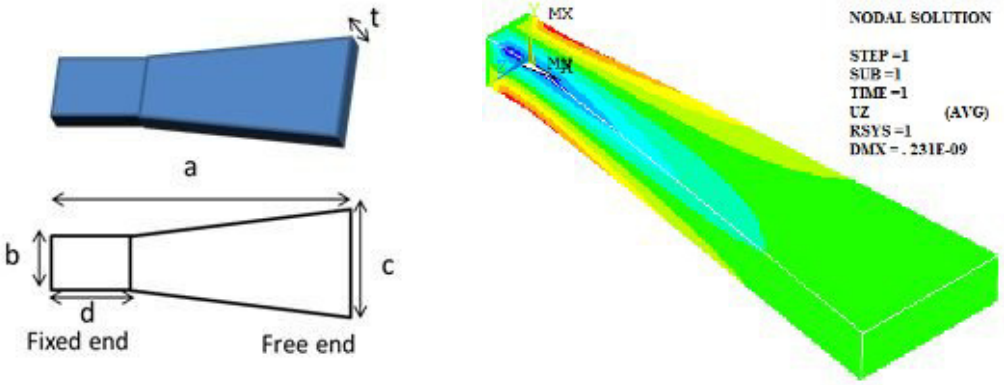

Fig. 4. (a) Second proposed microcantilever beam design; (b) It's free end deflection

3.3. Length wise symmetrical tree type microcantilever beam design

Alternative increment and decrement of width for different sections of rectangular microcantilever beam provide such type of microcantilever beam design, which is shown in Fig. 5(a). The length of each section is constant. Also the length and thickness of the complete beam are same as the conventional rectangular microcantilever beam. Parameter 'a' represents the length of each sections of the beam design. Parameter 'b' and 'c' represent the width of the odd and even number sections from the fixed end of the proposed microcantilever design, respectively. The value for parameter 'a', 'b' and 'c' is selected as 50 µm, 50 µm and 150 µm, respectively. The thickness 't' is 50 µm which is same as the conventional rectangular design.

Fig. 5(b) shows the deflection at the free end of this proposed microcantilever design with constant surface area (5,000µm^2) and pressure (19.2Pa). For the similar pressure the free end deflection of this length wise symmetrical tree type microcantilever design can be monitored as 0.213×10^{-9} m which is approximately twice as the rectangular beam free end deflection.

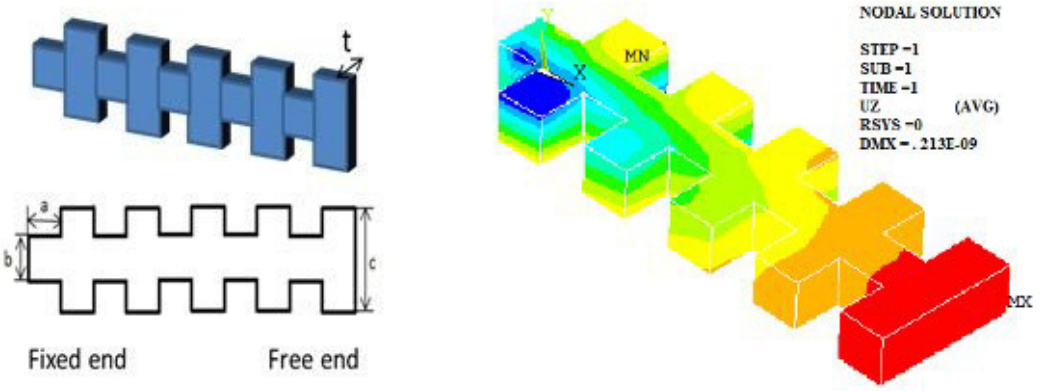

Fig. 5. (a) Third proposed microcantilever beam design; (b) It's free end deflection

4. Fabrication steps

Fabrication process of conventional and proposed microcantilever beam sensors have analyzed by the virtual fabrication FEM software Intellisuite. Basically fabrication steps involve introduction of silicon wafer (with crystal orientation 100) or substrate along with deposition of silicon di-oxide as a dielectric layer. The poly-silicon material has used for creating various designs of microcantilever beam. The beam surface geometry can be converted into required shape by using specific masks and sacrificial layer. Dry etching process has used for poly-silicon, dielectric layer and sacrificial layer etching.

5. Result Analysis

In triglyceride detection [4], the reaction between lipid and lipase alter the density of the de-ionized solution. The change in density causes change in pressure produced by the biomolecules and effects the free end deflection of the beam. The pressure 19.2 Pa which is equivalent to the surface stress 0.05N/m produces the free end deflection of 0.110×10^{-9} m for the conventional rectangular microcantilever beam. Same pressure produces 0.202×10^{-9} m, 0.231×10^{-9} m and 0.213×10^{-9} m deflection at the free end of first, second and third proposed microcantilever beam designs, respectively. Hence, the deflections for the proposed microcantilever designs are nearly 2× then the conventional rectangular microcantilever beam. Table 1 represents the deflection for the conventional rectangular and the proposed microcantilever beams with the same surface area (5,000μm^2) and constant pressure 19.2 Pa.

Table 1. Comparison Table

Beam type	Free end deflection
Rectangular design	0.110×10^{-9}m
First proposed design	0.202×10^{-9}m
Second proposed design	0.231×10^{-9}m
Third proposed design	0.213×10^{-9}m

In all these proposed designs, the deflection at the microcantilever free end increases because of large surface area at the free end of beam as compare to fixed end of beam. The bioreceptors attached at the microcantilever surface are more at the free end and bind almost all analyte molecules at the free end of beam. The biochemical reaction relatively large due to large number of binding at the microcantilever free end, which exhibits more deflection at the free end of all proposed designs as compare to conventional rectangular microcantilever beam. The rectangular

cantilever beam has the constant width along the beam length. While in the proposed microcantilever beam designs width increases linearly or non-linearly with respect to length. This gives the change in centre of mass of the beam. Because of the increment of width from fixed end to free end, the centre of gravity shifted toward the free end. Hence, small loading of biomolecules give measurable deflection at the microcantilever free end.

Fig. 6 shows the graph which represents the free end deflection of the rectangular and proposed microcantilever beams for various value of pressure generated by the surface biomolecules. The deflection curve for rectangular, first proposed, third proposed and second proposed microcantilever beam are denoted by **A**, **B**, **C** and **D**, respectively. This concluded that, with the same surface area (5,000μm^2) and same molecular pressure (19.2Pa) generated by analyte-receptor molecules, the proposed designs exhibit more deflection at free end and for the variation in molecular pressure the proposed designs are more sensitive than the conventional rectangular microcantilever beam.

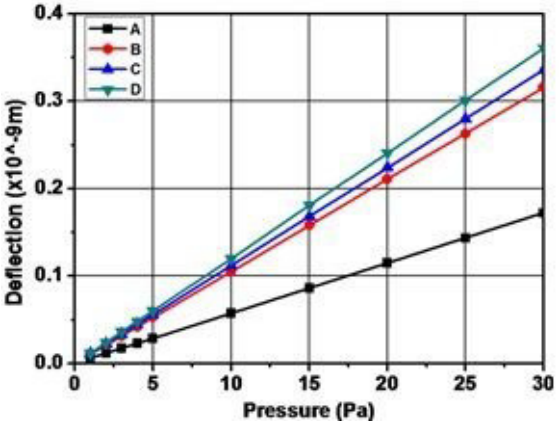

Fig. 6. Free end deflection verses applied molecular pressure

6. Conclusion

In ‘in vivo analysis’, rather than analyze the whole organism, experiment is done only on small cell, highly sensitive biosensors are required. These sensors should be able to convert small bimolecular activities or event into a measurable quantity. For such application, highly sensitive microcantilever beam designs with better deflection are analyzed in this paper. The study proposed three new microcantilever designs provide the free end deflection nearly 2× then the conventional microcantilever beam, while the beam surface area, complete length, thickness and pressure are same as the conventional microcantilever beam. The first, second & third microcantilever beam designs give the free end deflection 0.202×10^{-9}m, 0.231×10^{-9}m & 0.213×10^{-9}m, respectively. In our future work we will find the efficiency and sensitivity of these designs along with fractal surface for the detection of blood triglyceride.

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